Nonane

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.89	0.25	0.88	0.26	0.75	0.38

Model Results

Predicted value: 8.49 days

Global applicability domain: Inside

Local applicability domain index: 8.85e-01

Confidence level: 9.12e-01

Nearest Neighbors from the Training Set

Image not found
Nonane
Measured: 157
Predicted: 8.49

Image not found
Decane
Measured: 157
Predicted: 8.71

Image not found
Octane
Measured: 157
Predicted: 8.57

Image not found
Heptane
Measured: 88.3
Predicted: 7.54

Image not found
Undecane
Measured: 88.3
Predicted: 8.56